Antiferromagnetic long range order in the uniform resonating valence bond state on square lattice

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With extensive variational Monte Carlo simulation, we show that the uniform resonating valence bond state(U-RVB) on square lattice is actually antiferromagnetic long range ordered. The ordered moment is estimated to be $m \approx 0.17$. Finite size scaling analysis on lattice up to lattice size of 50×50 shows that the spin structure factor at the antiferromagnetic ordering wave vector follows perfectly the $\mathrm{S}_{\mathrm{q}=(\pi,\pi)} \simeq S_0 + \alpha(1/L)^{\frac{5}{4}}$ behavior, where L is linear scale of the lattice. Such a behavior is quite unexpected from the slave Boson mean field treatment or the Gutzwiller approximation of the uniform RVB state.

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The resonating valence bond(RVB) state plays an important role in our understanding of exotic physics in quantum antiferromagnet and the high T_c superconductors[1]. The RVB state is a quantum many body spin singlet constructed from coherent superposition of different pairing patterns of the spins on the lattice.

In practice, the most studied RVB states are those generated from Gutzwiller projection of Fermionic or Bosonic mean field state with condensed singlet pairs. It is well known that the RVB states generated from these two routes differ in their property qualitatively. For example, a Bosonic RVB state can be either short ranged in its spin correlation when the spinon excitation spectrum has a full gap, or , long range ordered when the Bosonic spinon condense. On the other hand, a Fermionic RVB state can have more choices for its spin correlation. Beside being short ranged with an exponentially decaying spin correlation, the spin can also choose to stay in various kind of critical states. For example, a Fermionic RVB state can have a large spinon Fermi surface or various kind of node structure in its spinon dispersion. The spin correlation in such critical state generally follows power law behavior. However, it is generally believed that it is difficult to describe state with long range magnetic order within the Fermionic RVB scheme without breaking the spin rotational symmetry. Such a difference between the Bosonic RVB state and the Fermionic RVB state stems from the fact that the magnetic long range order in the Bosonic RVB state actually originates from the condensation of the Bosonic spinon, while in the Fermionic RVB state, the Fermionic spinon must be paired before condensation. However, a condensation of triplet pair will inevitably break the spin rotational symmetry.

The relation between the Bosonic and Fermionic RVB state has been studied by many authors[10, 11]. It is found that when the RVB amplitude is extremely short ranged, or, extending only between nearest neighboring sites, and the lattice is planar, a Fermioinc RVB state can be transformed into a Bosonic RVB state with suitable redefinition of the RVB amplitudes. For Fermionic RVB state with longer range RVB amplitudes, their relation with Bosonic RVB state is still elusive. More generally, it is found that on the bipartite lattice, both Bosonic and Fermionic RVB state satisfy the well known Marshall sign rule for unfrustrated antiferromagnet, if they are both derived from a bipartite mean field Hamiltonian.

An analytical treatment of the RVB state is difficult. The most commonly adopted method to study the Fermionic RVB state is the slave Boson mean field theory. Beyond the mean field theory, there is also the more elaborate effective gauge field theory treatment[2–4]. However, it is well known that the mean field theory may fail qualitatively as the no double occupancy constraint is relaxed to a global one in such treatment. The gauge fluctuation correction, which can in principle improve the result of the mean field theory, are accounted for only at the Gaussian level in most cases and missed the singular gauge fluctuation effect at the lattice scale. As a variational state, the Fermionic RVB state is also studied by the Gutzwiller approximation[5], which try to estimate the effect of the local constraint by correcting the mean field expectation value with some correction factor. However, the Gutzwiller approximation can not produce any qualitatively different prediction from the mean field theory as to the spin correlation in the RVB state[6].

The variational Monte Carlo(VMC) method is a direct way to study the properties of the Fermionic RVB state. It is found that in certain cases the VMC result can be quite different from the mean field prediction. For example, on bipartite lattice, a well defined sign structure(the Marshall sign rule) may emerge out of a general mean field state through the Gutzwiller projection, even if the mean field state breaks the time reversal symmetry and has a complex valued wave function. Such a sign structure will restore the time reversal symmetry in the projected state and remove from the system possible topological degeneracy.

In this paper, we present another example in which

the mean field prediction is qualitatively changed by the Gutzwiller projection. We show the well know uniform RVB state on the square lattice with a large Fermi surface for the spinon actually describes a state with magnetic long range order.

The uniform RVB state first appears as a variational state for the high-Tc superconductors in Anderson's original paper on RVB theory of the cuprates[7]. The state has a large nested Fermi surface for the Fermionic spinon. Although it is later found that the d-wave RVB state is energetically more favorable than the uniform RVB state[8], the uniform RVB state is nevertheless still an interesting state of its own right.

At the mean field level, the uniform RVB state is described by a filled Fermi sea with a nested Fermi surface. The spin correlation function decays algebraically with distant as $\frac{1}{R^4}$. The spin structure factor at the antiferromagnetic wave vector is given by $S_{q=(\pi,\pi)} = \frac{3}{2N}$, in which N is number of lattice sites[9]. Thus at the mean field level, the uniform RVB state describes a state with no magnetic long range order. However, as the system presents a nested Fermi surface, the mean field state is instable with respect to infinite small perturbation toward antiferromagnetic ordering. Thus it is highly possible that the Gutzwiller projection may induce finite antiferromagnetic order in the uniform RVB state, in a way that the spin rotational symmetry remains intact.

The uniform RVB state is given by the Gutzwiller projection of the ground state of the following mean field ansatz

$$\mathrm{H}_{U-\mathrm{RVB}} = -\sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + h.c.), \tag{1}$$

whose mean field dispersion is given by $\epsilon_{\mathrm{k}} = -2(\cos \mathrm{k}_x + \cos \mathrm{k}_y)$. The uniform RVB state can then be written as

$$|U-\mathrm{RVB}\rangle = \mathrm{P_G} \prod_{\mathrm{k}<\mathrm{k_F}} c^\dagger_{\mathrm{k}\uparrow} c^\dagger_{-\mathrm{k}\downarrow} |0\rangle, \tag{2}$$

where $\mathrm{k_F}$ denotes the Fermi momentum of the spinon and is determined by $\epsilon_{\mathrm{k_F}} = 0$. $\mathrm{P_G}$ denotes the Gutzwiller projection into the subspace of no double occupancy. The state can also be written in the form of condensed pairs,

$$|U-\mathrm{RVB}\rangle = \mathrm{P_G} \left(\sum_{i,j} a(i-j) c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} \right)^{\frac{N}{2}} |0\rangle, \tag{3}$$

in which $a(i-j) = \sum_{\mathrm{k}<\mathrm{k_F}} e^{i\mathrm{k}\cdot(i-j)}$. Due to the bipartite nature of the square lattice, it can shown that the uniform RVB state satisfy the Marshall sign rule for a unfrustrated antiferromagnet[10, 12]. More specifically, the wave function of the uniform RVB state in a Ising basis is real up to a global phase factor and its sign is given by $(-1)^{N^A_\downarrow}$, where $N^A_\downarrow$ denotes the number of down spins in A sublattice.

To detect possible magnetic long range order in the uniform RVB state, we focus on the spin structure factor at the antiferromagnetic ordering wave vector

$$S_{\mathrm{q}=(\pi,\pi)} = \frac{1}{N^2} \sum_{i,j} e^{i\mathrm{q}\cdot(i-j)} \langle S_i \cdot S_j \rangle. \tag{4}$$

At the mean field level, the spin structure factor can be found to be given by $S_{q=(\pi,\pi)} = \frac{3}{4N}$. On the other hand, when the no double occupancy constraint is enforced by the Gutzwiller projection, the result is quite different.

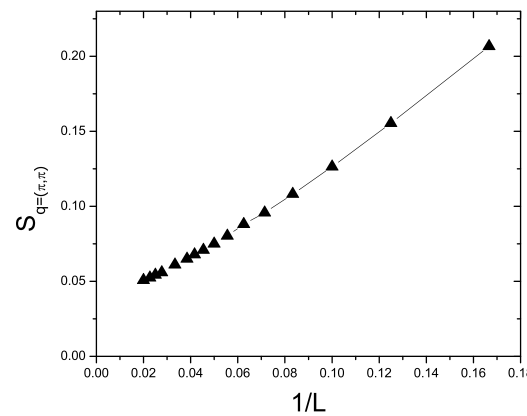

FIG. 1: The spin structure factor of the uniform RVB state at q $= (\pi, \pi)$ on a $L \times L$ square lattice as a function of the inverse linear scale of the lattice, $1/L$. Presented in this figure is the results for $L = 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 30, 36, 40, 44$ and 50. Periodic-antiperiodic boundary condition is adopted in the calculation to satisfy the closed shell condition. The error bars are smaller than the size of the symbols.

In Figure 1, we show the VMC result for the spin structure factor for lattice with size up to 50×50 as a function of the inverse linear scale of the lattice, $1/L$. In our calculation, we have used the periodic-antiperiodic boundary condition to satisfy the closed shell condition. We have used up to 4×10^6 statistically independent samples to estimate the spin structure factor. Each sample is drawn from the Markov chain with N steps of local updates. The statistical error estimated from the data is smaller than the size of the symbols in the figure. The spin structure factor of the uniform RVB state clearly extrapolates to a finite value in the thermodynamic limit.

To see the trend of the spin structure factor more clearly, we fit the data with the formula $S_{q=(\pi,\pi)} = S_0 + \alpha(1/L)^\beta$. The best fit to the data is found to be $\beta = \frac{5}{4}$ and $S_0 = 0.038$. Thus the ordered moment in the uniform RVB state is given by $m = \sqrt{S_0} = 0.17$, which is quite considerable as compared to the prediction of the spin wave theory for the Heisenberg model on square lattice. In Figure 2, a linear fit to the spin structure with

$(1/L)^{\frac{5}{4}}$ as the coordinates is shown. The linear fit is seen to work extremely well from the smallest lattice we have studied (6×6) directly to the largest lattice 50×50.

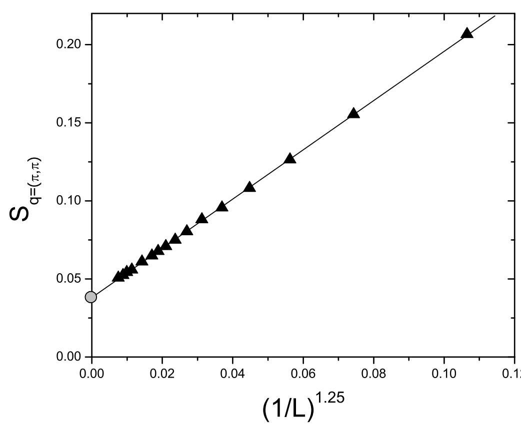

FIG. 2: The spin structure factor of the uniform RVB state at q $= (\pi, \pi)$ on a $L \times L$ square lattice as a function of $(1/L)^{\frac{5}{4}}$. Presented in this figure is the results for $L = 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 30, 36, 40, 44$ and 50. Periodic-antiperiodic boundary condition is adopted in the calculation to satisfy the closed shell condition. The gray dot on the y-axis denotes the fitted value of S_0. The error bars are smaller than the size of the symbols.

As a comparison, we also present the spin structure factor of another well known Fermionic RVB state on square lattice, namely, the π flux phase in Figure 3. The π-flux phase is generated by the following mean field ansatz

$$\mathrm{H}_{\pi-flux} = -\sum_{\langle i,j \rangle, \sigma} (e^{i\phi_{i,j}} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c.), \quad (5)$$

in which the phase factor $\phi_{i,j}$ is introduced to guarantee that each plaquette of the square lattice is threaded by a $U(1)$ flux of value π. In the π-flux phase, the spinon has a Dirac type linear dispersion and the mean field spin correlation also decay with distance as $1/R^4$. After the Gutzwiller projection, the spin correlation of the system is greatly enhanced. But as is clear in Fig.3, the π-flux phase does support an antiferromagnetic long range order. In fact, a finite size scaling analysis shows that the spin structure factor decays as $1/L^{\frac{3}{2}}$ with the linear scale of the lattice and extrapolates to zero in the thermodynamic limit(Fig. 4).

From these data, it is clear that uniform RVB state indeed describes a state with antiferromagnetic long range order. This is quite unexpected from the mean field theory and it represents the first example of Fermionic RVB state with magnetic order. Such a order does not originate from the condensation of spinon as in the Bosonic RVB state and respect the spin rotational symmetry. In

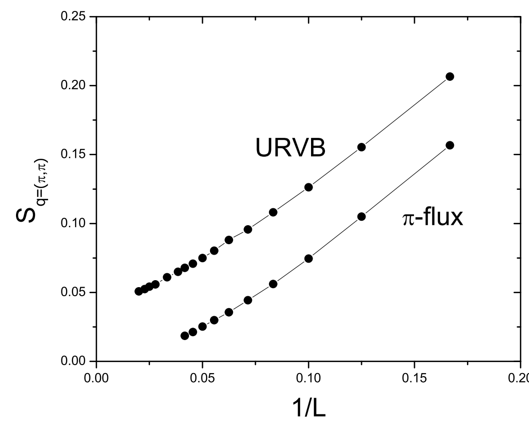

FIG. 3: The spin structure factor of the π-flux phase at q $=$ (π, π) on a $L \times L$ square lattice as a function of the inverse linear scale of the lattice as compared to the result of the uniform RVB state. Presented in this figure is the results for $L = 6, 8, 10, 12, 14, 16, 18, 20, 22$ and 24. Periodic-antiperiodic boundary condition is adopted in the calculation to satisfy the closed shell condition. The error bars are smaller than the size of the symbols.

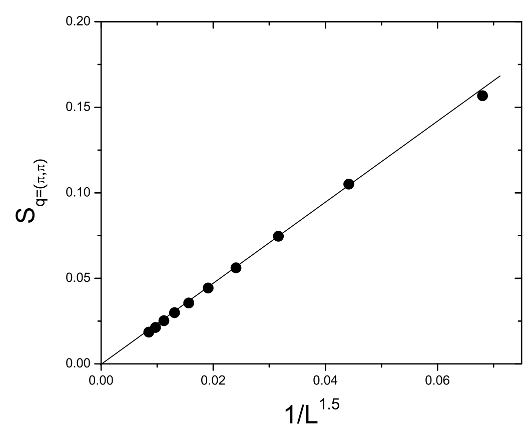

FIG. 4: The spin structure factor of the π-flux phase at q $=$ (π, π) on a $L \times L$ square lattice as a function of $1/L^{1.5}$. Presented in this figure is the results for $L = 6, 8, 10, 12, 14, 16, 18, 20, 22$ and 24. Periodic-antiperiodic boundary condition is adopted in the calculation to satisfy the closed shell condition. The error bars are smaller than the size of the symbols.

the uniform RVB state, the magnetic long range order can be understood as a result of the induced magnetic ordering in a system with nested Fermi surface.

Following the above reasoning, it is quite interesting to ask the following question: does the uniform RVB state have antiferromagnetic long range order in other spatial

dimension. In one dimension, the projected Fermi sea state is critical and the spin correlation function decay with distance as $\frac{1}{R}$, indicating no magnetic long range order. This can be taken as the result of the strong quantum fluctuation in one dimensional system. As fluctuation becomes weaker in higher spatial dimension, it is quite possible that the uniform RVB state in three dimension(on cubic lattice) also have antiferromagnetic long range order. A study of this issue, which is numerically quite demanding for large lattice, will be presented in a separated paper.

We note a recent preprint[13] independently confirmed the results of this manuscript.

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[1] P.W. Anderson, Mater. Res. Bull. 8, 153(1973).
[2] P.A. Lee, N. Nagaosa and X-G Wen, Rev. Mod. Phys. 78, 17 (2006); X. G. Wen, Phys. Rev. B 65, 165113(2002).
[3] C. Mudry and E. Fradkin, Phys. Rev. B 50 (1994) 11409, C. Mudry and E. Fradkin, Phys. Rev. B 49 (1994) 5200.
[4] Don H. Kim and P.A. Lee, Annals of Physics 272, 130 (1999).
[5] F.C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. 1, 36 (1988); T. Hsu, Phys. Rev. B 41 11379, (1990).
[6] Balázs Hetényi, Hans Gerd Evertz, and Wolfgang von der Linden, Phys. Rev. B 80, 045107 (2009). Balázs Hetényi, Phys. Rev. B 82, 115104 (2010)
[7] P. W. Anderson, Science, 235, 1196(1987); G. Baskaran, Z. Zou and P. W. Anderson, Solid State Commun. 63, 973 (1987).
[8] I. Affleck and J. B. Marston, Phys. rev. B 37, 3774(1988); G. Kotliar and J. Liu, Phys. Rev. B 38, 5142 (1988).
[9] D. P. Arovas and A. Auerbach, Phys. Rev. B 38, 316(1988).
[10] S. Yunoki and S. Sorella, Phys. Rev. B 74, 014408 (2006).
[11] N. Read and B. Chakraborty, Phys. Rev. B 40, 7133 (1989).
[12] Tao Li and Hong-Yu Yang, Phys. Rev. B 75, 172502 (2007).
[13] Y. Zhang, T.Grover and A.Vishwanath, arXiv:1102.0350.